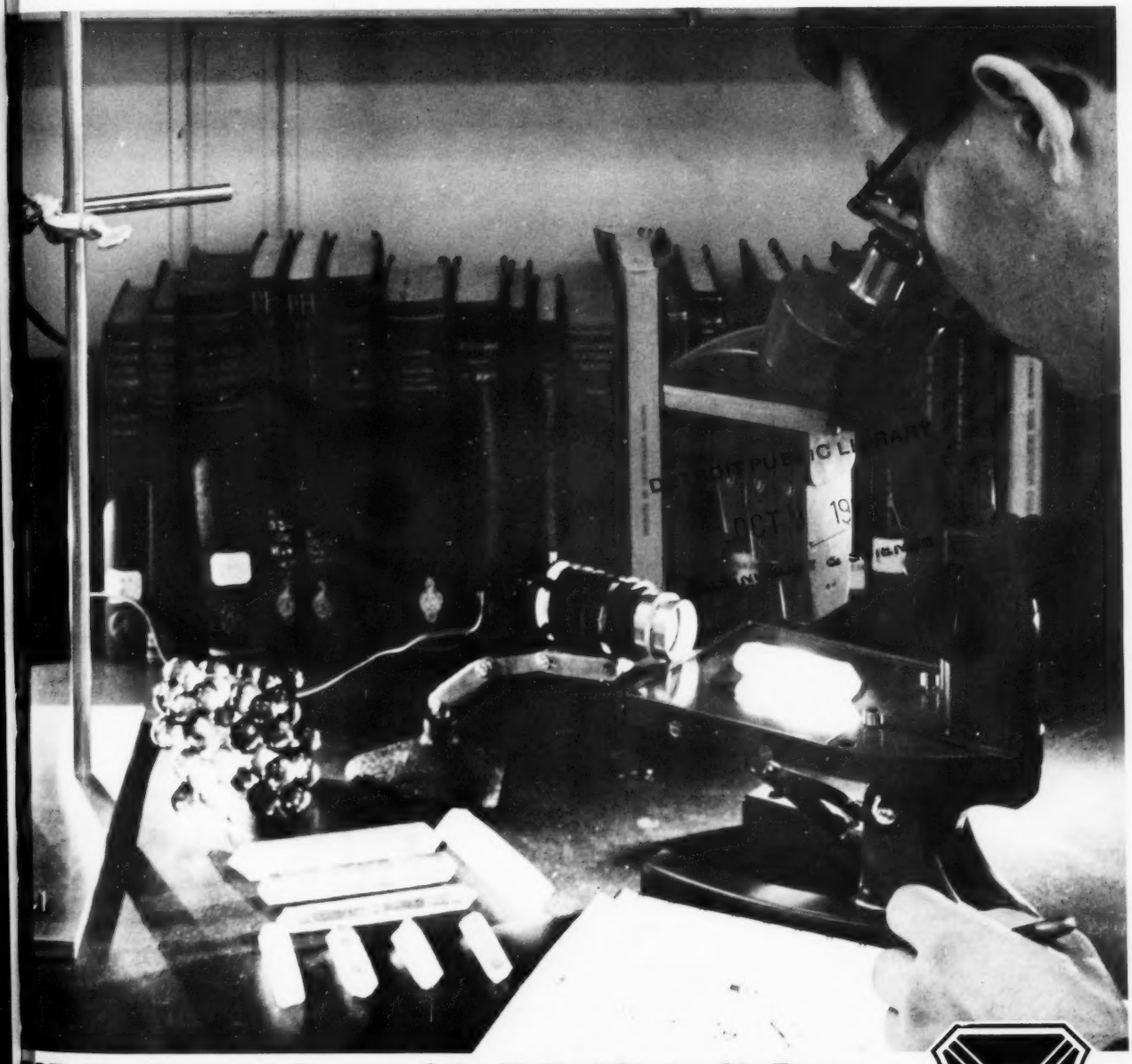
OAR RESEARCH REVIEW

OFFICE OF AEROSPACE RESEARCH ★ UNITED STATES AIR FORCE



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ON THE COVER:

Crystal analysis is an intrinsic part of solid-state research. AFCRL has facilities for analyzing crystals by the Mössbauer and Hall effects, X-ray diffraction, and electrical diffraction plus a variety of spectroscopic techniques. Here Carl A. Pitha of AFCRL is studying simple crystal dislocations.

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JACOB SEIDEN *Editor*

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THERMAL DIFFUSION AND STRUCTURAL ORDER IN LIQUIDS

JULIUS G. BECSEY and DR. JAMES A. BIERLEIN
Chemistry Research Laboratory, ARL

Thermal diffusion—the migration of molecules in a temperature gradient—is an interesting phenomenon which, apart from its value for the practical separation of materials, also yields information on the structure of the liquid state. Since the effect is very sensitive to the strength and range of intermolecular forces, it is a stringent test of any theoretical model of a fluid. Some recent studies at ARL on thermal diffusion in electrolyte solutions are directed toward developing a better understanding of molecular organization in liquids.

In accordance with the picture of ionic solutions first proposed by Eastman (1) and later elaborated by Frank and Wen (2), thermal diffusion is related to structural changes in the solvent induced by the electrostatic field of the solute. In this model, the solvated ion is surrounded by a zone of influence within which the solvent molecules are oriented by the electric field but can move relative to the ion. This secondary shell experiences a continuous change as the ion moves in the solvent; the solvent molecules are subject to an increasing degree of alignment as they enter the secondary shell and later relax by random orientation. For example, Fig. 1 shows a schematic representation of an aqueous ionic solution. In this picture the water is in a totally random state without interacting forces, a case which is probably never attained in reality. However, this situation is approximated by an ionic solution at a high temperature. The solvated ion, marked with a black circle, will create some degree of order in this randomly oriented water by virtue of its electrostatic field, and will build up a secondary hydration shell. When this ion makes a jump by diffusion from its original site to some terminal site, an energy E_1 will be absorbed by the solvent as the ion is released: this energy is required to collapse the secondary hydrate shell (order → disorder). The same amount of energy E_1 will be liberated at the terminal site, where a new secondary hydration shell is formed (disorder → order). If there is a temperature gradient in the solution, the ion will tend to migrate towards the cold region, because in this way it can get rid of the excess E_1 energy associated with the continuous reformation of the secondary shell. This corresponds to a positive heat of transport Q* carried by

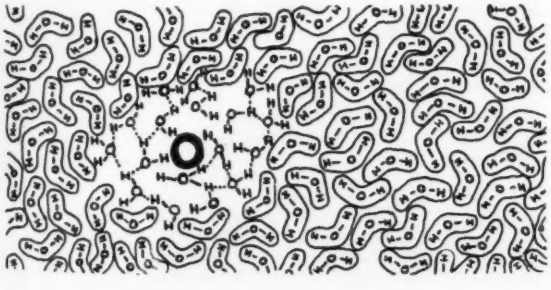

Figure 1.—Local structure near an ion.

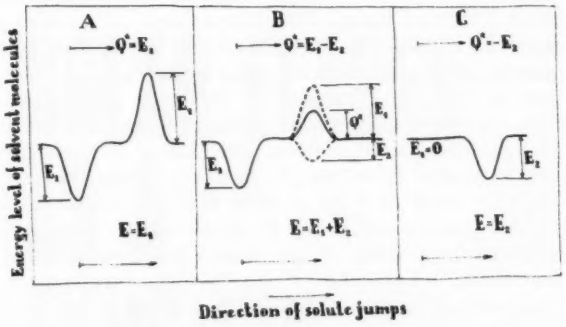

Figure 2.—Energy conditions in diffusion.

the ion in addition to the first-law heat flow. The energy conditions associated with the jump are shown in Fig. 2A. The heat of transport Q* is equal to E_1. Following the theory of Wirtz (3), if one increases the structural order in the solvent matrix (for example, by lowering the temperature of the solution), an additional energy E_2 will be needed to open up a hole in the solvent lattice. At the same time, E_1 will decrease somewhat because the solvent molecules adjacent to the ion will tend to resist reorientation by the ionic field and thereby act to squeeze out the ion to some extent. Thus, the heat of transport carried by the ion will be the difference of these two terms: $Q^* = E_1 - E_2$, where E_1 is the energy which is needed to dislodge the ion from its original site and E_2 is the energy which is required to open up a hole at the terminus of the jump (Fig. 2B). The total energy of activation is $E = E_1 + E_2$. Fig. 2C shows the limiting case $E_1 = 0$, in which the ionic field is insignificant compared to the intermolecular forces characteristic of the pure solvent: all the activation energy is consumed in forming a hole at the terminal site of the jump. This corresponds to a high negative heat of transport and to net ionic migration in the direction of increasing temperature. Hence Q* for a given solute is related to the inherent structural energy of the solvent. In dealing with two solvents which differ only in their isotopic composition, such as ordinary water and heavy water, it is reasonable to suppose that differences in heats of transport (with a given solute) arise almost entirely from a difference in the degree of intermolecular organization within the two liquids. For example, the heats of transport of several electrolytes studied were found to be considerably lower in deuterated water than in ordinary water (4). On this view,

therefore, our results in these solutions are explicable in terms of the more organized structure of heavy water compared with ordinary water. These data are consistent with the evidence put forward by other investigators that heavy water indeed has "more structure" than ordinary water.

These ideas can be extended and generalized to compare liquids of different chemical structure. Following the theory of Wirtz, we define the ratio $\Phi = E_1/E = \frac{1}{2}\left[1 + \frac{Q^*}{E}\right]$ as a characteristic quantity to express the change of energy at the initial site of the jump, normalized to the total activation energy (5). The parameter Φ provides a scale for ranking liquids in order of innate structural energy, ranging between $\Phi = 1$ (no molecular interaction) and $\Phi = 0$ (completely rigid structure). As a test of this idea, we have determined Φ experimentally as a function of concentration for solutions of alkali halides in formamide and its methyl derivatives (5). By extrapolating to infinite dilution, values of Φ are obtained which are characteristic of the pure solvent. Using KI as a common solute, we obtained large values (nearly unity) for Φ in dimethylformamide, and therefore we classify this solvent as nearly structureless. Formamide and methylformamide are found by this criterion to be much more highly ordered ($\Phi = 0.6$). These results probably can be ascribed to hydrogen bonding as the structural force acting in the solvent matrix. For example, heavy water has more structural order than ordinary water, due to the higher degree of hydrogen bonding, and methylformamide and formamide also have more structure than dimethylformamide for the same reason.

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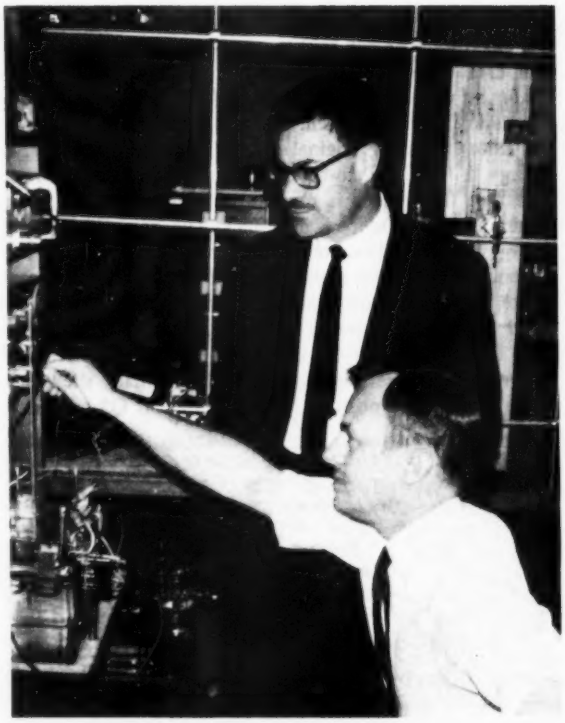
Dr. James A. Bierlein has been with ARL since 1950, and became head of ARL's Chemistry Research Laboratory in 1956. He received a B.S. in Chemistry from Purdue University in 1942 and, except for periods of study, has been associated with the Air Force ever since, either as an officer or as a civilian employee. Dr. Bierlein is a 1945 graduate of the Army Air Force Engineering School, and took his M.S. and Ph. D. degrees in Chemical Engineering from the Ohio State University in 1948 and 1951, respectively. In 1962 he was a postdoctoral fellow in physical chemistry at Cambridge University. During 1966-67 he served a 15-month tour of duty with the Office of Naval Research, London, as Director of the Sciences Division.

Mr. Julius G. Becsey joined the Chemistry Research Laboratory at ARL in 1964, having been employed there as a research associate of the Ohio State University Research Foundation since 1961. He is studying transport phenomena in liquids, particularly thermal diffusion and diffusion in solutions. Before coming to ARL, he was a research chemist for the National Cash Register Company. Mr. Becsey received an M. S. degree in Physical Chemistry from the University of Budapest in 1955, and worked as a research chemist for the Hungarian Telecommunication Research Institute until October 1956, when he left his native Hungary. He has a number of publications and two patents to his credit, and is a member of the American Chemical Society.



Dr. James Bierlein (standing) and Mr. Julius Becsey measuring electrical conductivity of diluted electrolyte solutions.

SOLAR FLARES AS A FUNCTION OF SUNSPOT SIZE

Solar flares, the giant bursts of solar matter that erupt out to altitudes of 75,000 miles or so within a few hours, create disturbances that can seriously affect communications, surveillance, and space operations.

Flares are associated with sunspots and they probably occur only when sunspots are present. But not all sunspots—or, more precisely, sunspot groups—produce solar flares. The question naturally arises as to whether the occurrence of solar flares can be correlated with the size and growth pattern of particular sunspot groups in a forecasting scheme.

AFCRL, in cooperation with the Air Weather Service (AWS), is investigating this possibility. The study is part of a broader program at AFCRL devoted to environmental forecasting, the forecasting of all naturally occurring phenomena in the upper atmosphere and the near-space region that might affect Air Force operations. All phenomena of interest under this program—airglow and auroral intensity, geomagnetic disturbances, solar proton showers, and so on—are closely associated with solar activity. Solar flares are the most violent of solar activities and the most unpredictable.

The AFCRL-AWS investigation has led to an objective technique for assessing the probability of a solar flare occurring in a particular sunspot group as a function of the size of the area covered by a sunspot group. Sunspots, it should be noted, tend to occur in clusters or groupings, with the groupings varying greatly in area. It is generally believed that large, rapidly growing, magnetically complex sunspot groups are the breeding grounds for solar flares. This belief has been difficult to verify objectively because of the lack of a sufficiently large and homogeneous data sample.

The data sample covers 10 years of information for the period 1955 through 1964. Sunspot data used in the study came from the Greenwich Observatory which, for almost a century, has published daily positions and areas of sunspot groups. Flare data were taken from observations made at AFCRL's Sacramento Peak Observatory at Sunspot, New Mexico. Sacramento Peak Observatory reported 11,245 flares during the 10-year period.

The AFCRL analysis resulted in a number of forecast tables. The AFCRL-AWS investigators divided all sunspot groups among 10 area categories. These area categories range from more than 1200 millionths to less than 30 millionths of the visible hemisphere. Tables were developed which show the probability of a flare occurring in a particular sunspot group in each category within a following 6-hour period. Large flares (of importance 2 or greater) have only a 0.1 percent probability of occurring during any following 6-hour period within small-area sunspot groups. But there is a 9.8 percent probability of a large flare occurring in groups with areas greater than 1200 millionths of the sun's hemisphere. Smaller flares, of course, occur much more frequently. For flares of all sizes, the probabili-

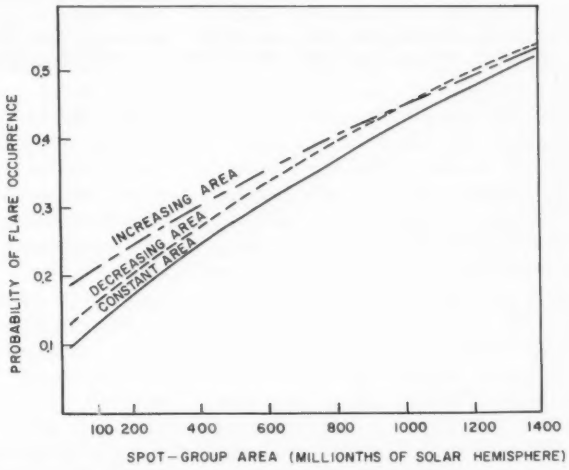


Figure 1.—Probability of flare occurrence versus area of sunspot group.

ties are 17.6 and 50 percent, respectively.

Are flares more likely to occur in sunspot groups that are increasing in area size, as is generally believed? Yes, but only slightly. Curiously, there is a slightly greater probability (about 1 percent) of a flare occurring in areas that are either increasing or decreasing in size than there is in sunspot groups maintaining a constant area. The study shows that a sunspot-group area remains relatively stable during any 2-day period. About 60 percent of the 17,845 sunspot groups identified over the 10-year sample remained in the same area category from one day to the next. The other 40 percent were divided about equally between increasing and decreasing area groups.

The AFCRL-AWS investigators conclude that, although there is only a slightly greater probability of a flare occurring in a sunspot group that is either increasing or decreasing in size, this knowledge does add useful forecast information.

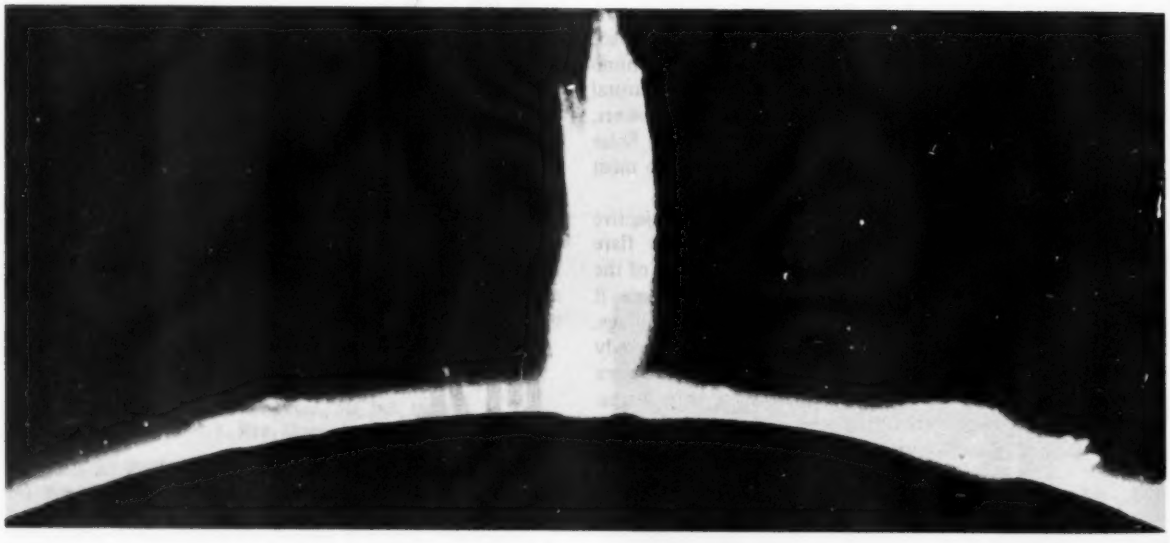


Figure 2.—Typical flare taken at AFCRL's Sacramento Peak Observatory using a coronagraph which produces an artificial eclipse.

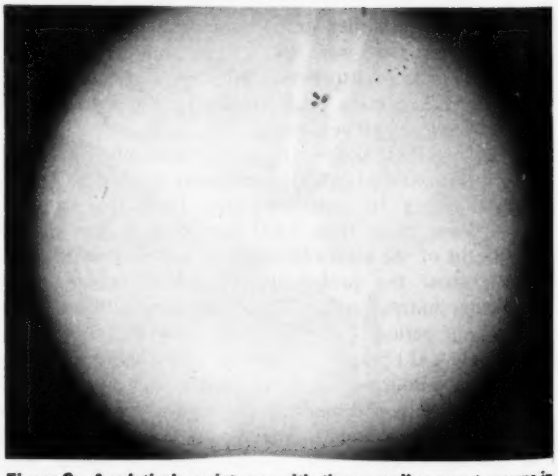


Figure 3.—A relatively quiet sun with three small sunspot groups in the northern hemisphere.

over-the-horizon radars: historical context

RESEARCH INFORMATION OFFICE, AFCRL

Over-the-horizon radars have been much in the news lately. In testimony before the Senate Armed Services Committee, Dr. John S. Foster, Jr., Director of Defense Research and Engineering, noted that "We already are countering the (Soviet Union's Fractional Orbital Bombardment System) effort by installing new over-the-horizon radars to provide adequate warning for our alert bombers." Former Defense Secretary Robert S. McNamara also said in recent testimony, "In order to provide a backup for BMEWS (Ballistic Missile Early Warning System), we have already deployed several over-the-horizon (forward-scatter) radar transmitters and receivers . . . We presently plan to begin installing the first backscatter OTH radar in the near future."

Both the forward-scatter and backscatter over-the-horizon systems detect the ionospheric disturbances associated with the missile launch. In the forward-scatter system the transmitter, facing a receiver thousands of miles away, continuously reflects (scatters) a signal from the ionosphere in the forward direction. When the ionosphere is disturbed by a missile passing through it, the disturbance is detected as a perturbation in the signal reaching the receiver. In the backscatter system, the radio energy from the transmitter is scattered back from the ionospherically disturbed region in the direction of the transmitter and is detected by a receiver located at, or near, the point of transmission.

Many companies and agencies have contributed to over-the-horizon systems—the Radio Corporation of America, Rome Air Development Center, the Naval Research Laboratory, General Electric, and others. Progress is marked through such project designations as COZI, Madre, Tepee, CAME BRIDGE, and so on, and by several score key research papers dealing with improved radar componentry and the general properties of the ionosphere. Nevertheless, the trunk of the geneological tree and one of the two major branches—the forward-scatter system—consist of work that was originated and carried forward by AFCRL.

The originator of the concept of detecting an artificially disturbed ionosphere by radar was Dr. Philip Newman of AFCRL. The concept, beginning in 1946, led to a long series of contracts with Raytheon to develop ionospheric probing radars and systems techniques. Initially, this work was concerned with generalized techniques and not with missile-launch detection systems. But, in the mid-1950's, a group at AFCRL under Wilbur H. Vance began to examine these techniques as a possible basis for a true long-range launch-detection capability, one that would overcome the line-of-sight and geographical limitations of BMEWS.

From these studies, it was concluded that the ionospheric disturbance should be detectable at long ranges, either by forward-scatter or backscatter techniques. Over-the-horizon detection could provide a 30-minute warning as against about 15 minutes for BMEWS. AFCRL pursued both approaches, the forward-scatter work being done primarily in-house, with the backscatter work on contract to Raytheon. Preliminary experiments involved the detection of launches over the Atlantic Missile Range.

This successful work led the Director of Defense Research and Engineering in 1960 to ask AFCRL to undertake a crash program to evaluate the forward-scatter technique in a simulated operational environment. This program was designated Project CAME BRIDGE. Transmitter sites were established in Hawaii and Midway Island in the Pacific, with six receiving sites ranging from Labrador to Panama. The test targets were missiles launched from Vandenberg AFB in California. All sites were contractor-operated, except for the master receiving site at Bedford, Mass., operated by AFCRL. Each site made continuous recordings of signals received from the transmitters, and magnetic-tape data were sent to AFCRL for reduction and analysis. Processed data were analyzed and "detections" were identified without knowledge of the actual time of missile launchings. By this means statistical measures were obtained for such operational parameters as reliability of detection, false alarms, warning time, and so on.

The effort of an entire AFCRL laboratory under Vance was devoted to the experimental systems for a four-year period. The decision to undertake the present operational system was based on the demonstrated high performance of the AFCRL experimental system. Following the large-scale test program, operational system parameters were established by AFCRL and the program was then transferred to the Electronic Systems Division, AFSC, for systems development. AFCRL has continued to serve as a consultant for both the forward and backscatter systems.

a survey of coding theory in the Soviet Union

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"The field of coding theory is by now well established as an important aspect of information theory. Its direct applications to the enhancement of communication and computing systems are potentially very great, and in practice are increasing rapidly after a rather slow beginning. Moreover, the principles and theoretical results that form the core of coding theory have exerted a significant effect upon the growth of information theory itself and, to a lesser extent, upon developments in several peripheral fields linked to coding theory through common language, techniques, or applications: switching theory, including some aspects of computer organization and computer memory design, the design of statistical experiments, group theory, pattern recognition, automata theory, and reliability theory. Contributions to coding theory, measured in terms of the number of technical papers published each year in the U.S. on the subject, have been steadily increasing for the past decade."

The above paragraph introduces the first comprehensive U.S. survey of Soviet research in coding theory. This survey was recently completed by William H. Kautz and Karl N. Levitt of the Stanford Research Institute under the sponsorship of the AFOSR Directorate of Information Sciences. (1) The principal investigators had found, in conjunction with their work in the Institute's Computer Techniques Laboratory, that many Soviet contributions to this field were not well known in the West. Moreover, many papers that have been translated go unnoticed because they appear in unlikely journals, appear several years later than the original publication, are not properly classified for retrieval, or are of poor quality for comprehension. Results are often obscured by mathematical notations or are written in a style even good translation cannot overcome. Whereas the Soviet abstracting and announcement service (the All-Union Institute of Scientific and Technical Information, VINITI), and the translation and republication service (Izdatelstvo Inostrannoi Literatury) have brought U.S. publications to the attention of Soviet researchers, as reflected in their citations to U.S. literature and in their low incidence of duplication of published technical results, Kautz and Levitt have found Soviet contributions predating equivalent U.S. results and an apparent lack of awareness by U.S. researchers of Soviet work. Of equal gravity, Kautz and Levitt find that their assessments differ from those of two recent U.S.-made surveys. This they attribute to the sporadic literature coverage of these prior efforts.

The Kautz-Levitt survey is in three parts. The first summarizes new technical results in coding theory, as well as conclusions that can be drawn from them with respect to areas of competence. The second part, constituting the major portion of the report, provides details of numerous technical results, organized under the following subject headings:

- history and origins of coding theory in the Soviet Union;
- random coding methods;
- bounds on random error-correcting codes;
- construction of random error-correcting codes;
- cyclic codes;
- the structure of codes;
- burst- and erasure-correcting codes;
- asymmetric-channel codes;
- deterministic decoding techniques;
- probabilistic decoding techniques;
- codes for computation and computer applications;
- noiseless-channel coding;
- synchronization codes;
- unit-distance codes (Gray codes);
- pseudorandom sequences and code rings;
- evaluation of coding systems; and
- other coding applications.

The authors have specifically excluded considerations of coding that are aspects of computer programming (i.e., "coding" a problem for a computer); genetic, chemical, linguistic, and legal interpretations of the term "coding"; and uses of simple codes for such purposes as pulse-code modulation, analog-to-digital converters, and edge-punched cards. An appendix lists several specialized and frequently mistranslated terms that appear in titles of Soviet papers. The third part is the bibliography that is subdivided into a section alphabetic by first author; a list of periodicals, aperiodicals, etc. appearing more than a few times in the bibliographic citations; and a list of references, alphabetic by first author, to non-Soviet items referred to in the text.

Kautz and Levitt report that Soviet work on the theory of error-correcting and other codes was almost nonexistent prior to 1957. Today's level of effort is only slightly behind that in the West in both quality and quantity. Many early papers were based on Shannon's 1948 report and those of his followers. The authors find no Soviet advances comparable to Slepian's discovery of group codes, the Bose-Chaudhuri-Hoquenghem multiple-error-correcting codes, and probabilistic decoding (Wozencraft). They do find that Soviet efforts frequently provide contributions that help to complete the body of knowledge constituting coding theory. The strongest areas of Soviet research are in noiseless coding; the synthesis of decoders for cyclic error-correcting codes, particularly majority decoders; asymmetric-

channel codes; random coding bounds; and various application criteria. Conspicuously lacking in the Soviet literature is work on pseudorandom sequences; good cyclic codes; implementation of sequential decoding algorithms; and applications of codes to such practical problem areas as information retrieval, redundant computer design, and memory access switches.

Kautz and Levitt believe that the only significant difference between Soviet and U.S. work in coding theory is at a conceptual classificatory level. Coding theory in the U.S. is considered a branch of information theory. It derives its practical motivations primarily from radio and wire communications, and secondarily from radar and computer applications. In the U.S.S.R., information theory is subsumed, with switching theory, automata theory, and studies in other disciplines ranging from economics to artificial intelligence, under the umbrella term, "cybernetics."

Kautz and Levitt identify some 20 unsolved problem areas suggested directly or indirectly by Soviet coding research. These are in addition to those contained in a 1961 paper by R. L. Dobrushin, most of which remain unsolved.

The authors note that most of the published papers of Soviet research can be expected to be reported in six technical journals and two abstract journals, all but one of which are regularly translated into English. They observe that, though proceedings of symposia (that have been held annually for the past several years) are formally announced, they are not widely publicized. They suggest that the quality of translations be improved. They found it necessary on occasion to obtain original-language papers when deficiencies in translations could not be overcome by an awareness of common types of mistranslation.

This study has a value beyond its obvious contribution to U.S. researchers in coding theory and its applications. It has broader import for the phenomenon often called the "information explosion." Kautz and Levitt have painstakingly surveyed and evaluated over 400 papers appearing between 1960 and March 1967. Their 1 document is a guide to far more literature than most researchers would have the time to digest, even if they could acquire it. Moreover, they have highlighted deficiencies in the quality of the literature as it is packaged for U.S. consumption. The review article is not a new device for overcoming the "information explosion"; but it may perhaps not be widely recognized as such by individuals both within and outside the information field. That it can be such is ably demonstrated by Kautz and Levitt. They also commented on review articles that failed to meet this mark. It is believed that the dilemma created by the "information explosion" could be appreciably ameliorated through the wise use of this review device. The "wisdom" factor, however, *must* be exercised both with respect to the selection of topic *and* investigators.

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determination of the zirconia-hafnia phase diagram

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Metallurgy and Ceramics Research Laboratory, ARL

Zirconia, ZrO_2, and hafnia, HfO_2, are very similar oxides and are characterized by excellent chemical stability and high melting points. Thus, a determination of the ZrO_2-HfO_2 phase diagram was of considerable practical importance for a number of reasons.

First, these oxides are usually associated in naturally occurring minerals in which zirconia is the major constituent and hafnia the minor constituent. Their separation is very difficult and expensive and, in fact, the separation processes have only been developed quite recently and are not applied commercially. Commercial grades of zirconia or hafnia each contain the other oxide as an impurity. For example, commercial zirconias contain approximately 2% hafnia. This being the case, a knowledge of the effects of these impurities on the properties of zirconia and hafnia was desirable.

A second reason for determining the zirconia-hafnia phase diagram was that, with the good refractoriness and chemical stability of both oxides, a potential existed for one or more excellent intermediate compositions. In addition, a knowledge of this system could act as a broad foundation for the investigation of new multicomponent systems based on ZrO_2 and HfO_2. It was for these reasons that a comprehensive investigation of the system was initiated.

The similarities of zirconia and hafnia can be illustrated by their crystal structures and polymorphy. At low temperatures both oxides have a monoclinic structure in which the lattice parameters differ by less than 0.5%. Both transform to a tetragonal structure on heating, the inversion temperature for zirconia occurring at approximately 1,050°C and that of hafnia at approximately 1,700°C. The inversions occur over a temperature range rather than at a given temperature and there is a hysteresis observed, i.e., the inversion occurs at a higher temperature on heating than on cooling. The tetragonal structures are very similar also, with lattice parameters differing by approximately 1.0%. With a further increase in temperature both oxides undergo a second inversion, which is a structural change from tetragonal to cubic. For zirconia, this inversion occurs at 2,285°C, while the temperature for hafnia is 2,700°C. The cubic structures are stable to the melting points, which

are 2,680°C for ZrO_2 and 2,900°C for HfO_2.

While similarities in properties are the rule, the two oxides differ greatly in their ability to absorb neutrons. Zirconia has a low neutron-absorption cross section and, in contrast, hafnia has a high neutron-absorption cross section. This difference is very significant for any applications involving nuclear energy.

The ZrO_2-HfO_2 system was studied by a number of different techniques to accurately establish the phase diagram. (1) Samples were annealed at and quenched from temperatures at regular composition and temperature intervals for the complete system. These samples were examined by metallographic, X-ray diffraction and electron-probe analyses. Results in all cases revealed complete solid solubility. X-ray lattice parameter studies revealed smooth curves with slight negative deviations from Vegard's law, thus giving further evidence for complete solid solution. Complete solid solubility was also indicated by melting-point determinations, which were found to lie approximately on a straight line connecting the end members. The monoclinic-tetragonal inversion was investigated by differential thermal and high-temperature X-ray analyses. A continuous increase in this inversion was found as the composition moved from ZrO_2 to HfO_2, thus offering further evidence for complete solid solution.

Based on this data, a phase diagram has been constructed and is presented in Fig. 1. All evidence indicates complete solid solubility, and a diagram of this type has been drawn. The melting-point determinations are plotted as triangular points and are assumed to lie approximately midway between the solidus and liquidus temperatures. A cubic-phase field has been included in the diagram since the tetragonal-cubic inversion has been reported in ZrO_2 by Smith and Cline (2) and in HfO_2 by Boganov, Rudenko and Markarov. (3) This area was not investigated in this work, however. The monoclinic-tetragonal inversion in the end members and the binary compositions have been presented, with the start and finish of both the heating and cooling inversion plotted. In the diagram, the circles denote the inversion on heating and the crosses denote the inversion on cooling. These points were obtained by a combination of differential thermal and high-temperature X-ray data.

In conclusion, the ZrO_2-HfO_2 system has been determined from 600°C to the liquidus temperatures. Results have revealed that there is complete solid solubility and a gradual change in properties rather than a compound or compounds formed superior to the end members. This gradual change minimizes the effect on properties of "impurity" amounts of one oxide in the other.

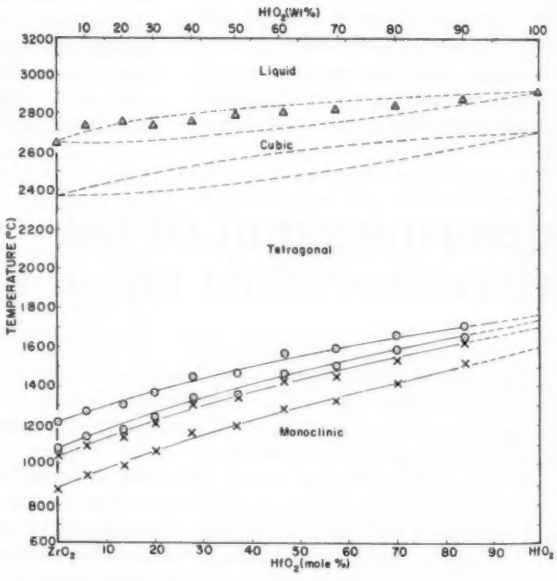

Figure 1.—The ZrO_2-HfO_2 System.

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MODELLING OF PLASMAS: ATOMISTIC AND COMPUTERIZED

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INTRODUCTION

Today, the major attention of theoretical physics is being pulled in two opposing directions: 1) the analysis problem—what, if any, are the "ultimate" elementary particles and their properties? and 2) the synthesis problem, with overtones for applications—since a material substance consists of many atomistic particles, how are the macroscopic observable properties of the material to be derived from the properties of the underlying, microscopic, unobservable atoms? Here, we are addressing ourselves to the latter, i.e. the many-body problem and, more specifically, to the contributions of a combination of large-scale digital computers and their associated displays to the solution of this problem. It turns out that these contributions are of a more fundamental nature than mere calculational simplification. Among the pioneers in this field are O. Buneman* and his associates at Stanford University.

A theoretical study of a material substance consists in devising a theoretical model of the substance. This demands a judicious balance between complexity and simplicity. The model must be complex enough to retain certain of the subtleties of the original, real substance, yet simple enough for these to be calculable from the model. An illustration is the model of a solid given in Fig. 1. It consists of a one-dimensional infinite array of identical molecules with a spring force between neighboring molecules. This model, although simple, has proved useful in calculating the specific-heat properties of solids.

Models of material substances can usually be classified into two categories: 1) atomistic, many-body and 2) phenomenological.

In an atomistic approach, a more detailed view is taken of the substance. The primary effort is focused on the individual molecules of a molecular model of the substance. One introduces the equations of motion for the individual molecules and solves these equations for their trajectories. This solution, known as the "microscopic" solution, is not satisfactory since the individual molecular trajectories are not directly observable experimentally. Thus, the essential task becomes one of obtaining an integrated mental grasp of all the individual trajectories—or at least of a significant portion—which is related to quantities directly observable in experiment. One illustration of such a unification of the trajectories is an averaging process over the individual trajectories. This leads to formulas presenting the space-time evolution of "macroscopic" quantities—i.e. directly, experimentally observable quantities such as temperature, density, etc.

On the other hand, in a phenomenological approach a simpler, less detailed view is taken of the substance. The macroscopic quantities are spread out continuously over space and are the items of original concern. The equations deal directly with these macroscopic elements; the solutions of the equations supply their space-time evolution directly. No microscopic intermediary intrudes.

Historically, the atomistic approach has been applied with mixed feelings. Even at the turn of the century a number of famous physicists deemed the introduction of atoms into theoretical investigations of material substances as an unnecessary and undesirable appendage. Eventually, however, the physical reality of atoms assumed an unassailable position in the world of physics, and the atomistic approach became the standard for the modelling of material substances. Yet, despite this atomistic victory, the phenomenological approach has remained the mainstay in specific non-equilibrium problems. The atomistic, many-body approach has been limited to equilibrium problems and to general theorems—e.g., the postulates necessary to derive the phenomenological Navier-Stokes equations in fluid mechanics from the Newtonian equations for the individual molecules.(1)

THE PROBLEM

The reason for this neglect of the atomistic, many-body approach lies in the attendant complexities in comparison to the phenomenological approach. Basically, the atomistic program is twofold—to determine the individual molecular trajectories, and to integrate them into a unified mental image. The point is, even if the individual trajectories could be calculated, the intricacies of attaining a macroscopic grasp of the trajectories of say 10^{12} particles encountered in matter are overwhelming. Thus, very often, the major stumbling block is said to be the hugeness of the number of particles.

Actually, the large number of particles only partly explains the difficulty. The feasibility of achieving a unified picture of the individual particle trajectories hinges more on the simplicity of the relationship between the individual trajectories than on the smallness of their number. Thus, the trivial example of three million molecules moving with equal velocities on equidistant parallel lines with equal phase differences presents a simpler situation than three particles in arbitrary motion.

Hence, the study of the atomistic, many-body problem can be reformulated into a twofold program: 1) to search for physically significant models with manageable relations be-

*Phases of the work have been supported by the Joint Services Electronics Program (U.S. Air Force, Army and Navy) at Stanford University.

Figure 1.—One-dimensional molecular model of a solid.

tween the particle trajectories; and 2) to seek more sophisticated techniques to tie the individual trajectories into a macroscopic package.

EARLY HISTORY

An early illustration of an atomistic model involving particle trajectories with manageable interrelations is found in a classic, didactic paper (2) written by Schrödinger* in 1914. In this paper, Schrödinger coped with a provocative challenge facing atomic theory at that time. If atoms existed physically—and in 1914 there were famous doubters—then an atomistic model ought to have made a difference when compared with the corresponding phenomenological model. One should have exhibited a theoretical study of a physical system in which the properties of the system calculated on the basis of the atomistic model contradicted those of the associated phenomenological model. Until this paper was presented, no such crucial contradiction had been known. Schrödinger met with success in his study of the atomistic model of Fig. 1, discussed above. The reason for his success was the particularly simple but nontrivial kinship among the trajectories of the individual molecules—the different integral orders of the Bessel function.

A decisive advance in handling atomistic models was made by Hartree and Nicolson (3) in the early 1940's with the introduction of computer modelling techniques. The writer of this article is unaware of the exact inspiration which triggered their approach. However, we can look upon their reasoning as being analogous to the reasoning behind wind-tunnel modelling. Much can be learned about airplane motions from small models in wind tunnels. Similarly, systems with a large number of molecules can be modelled by systems with fewer molecules. Thus, using a desk calculator, they studied a diode by following the motions of 30 electrons constrained to one dimension. There still remains the problem of a unified grasp of the individual trajectories. This is automatically resolved by sheer observation of a graphic display of all the trajectories as a single unit.

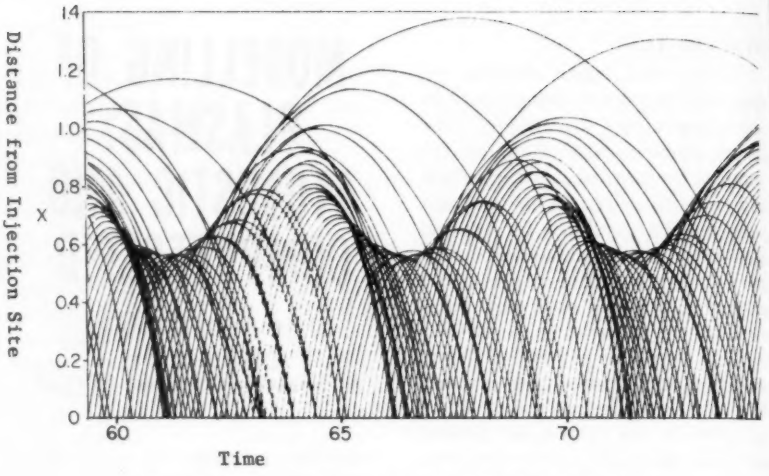

Figure 2.—Electron trajectories in an infinite diode (ref. 4).

How a graphic display accomplishes this macroscopic integration is illustrated in Fig. 2. This figure displays simultaneously the distance-versus-time trajectories of each electron in a diode of infinite extent. The electron motions are constrained to one dimension. It will be noted that each electron is injected with the same velocity and returns to the injection site. By simple observation, the display of the individual trajectories consolidates into the macroscopic picture—namely, a periodic oscillation of charge density both in time and depth of electron space penetration.

The next significant stage in atomistic computer modelling was the introduction of the large-scale digital computer and its associated displays, especially by O. Buneman and his co-workers during the last decade. Thus, atomistic computer modelling became established as a potent technique in diverse many-body problems, especially those concerned with plasmas* and including the evolution of astrophysical systems.

On the IBM 7090 computer it is practical to treat physically significant plasma models involving 10^4 charged particles if their trajectories are restricted to one dimension, and 10^3 particles if their trajectories are two-dimensional. However, no physically meaningful three-dimensional models appear feasible on this computer.

Here the reader may wonder as to what would permit a plasma containing, say, 10^{12} particles to be reliably modelled by 10^3 particles. The essence of the answer lies in the constraints imposed on the plasma. One barters the number of particles for the constraints. For example, for an isotropic plasma, a model of 10^{12} particles is equivalent to one with the cube root of 10^{12} particles—i.e., 10^4—if the particle trajectories are constrained to one dimension. More generally, the bartering becomes feasible if the constraint implies the existence of a typical volume element such that the details of the internal motions of the individual molecules within this volume intimate no macroscopic consequences. One can test this assumption by increasing the number of particles to determine if the results remain invariant.

To summarize the notion of atomistic computer modelling:

1) Atomistic computer modelling is a compromise between the full-fledged atomistic approach, where the path of each molecule counts, and the phenomenological approach where the particle motions are spread out continuously over space. Here it is still a particle approach; but, because of the reduced number of particles, the particle is coarser than a molecule.

A decade later, Schrödinger discovered quantum mechanics. One can see the germ of his discovery in his 1914 paper.

Reference 4 is a summary review article of computer modelling of plasmas.

Similarly, space and time are coarse-grained in discrete steps.

2) Computer modelling contributes to the solution of the core difficulty of the many-body problem—a unified grasp of the individual trajectories—by a reduction of the number of particles and the integrated display of the trajectories. Such atomistic models with a reduced number of particles are permissible for many-body problems with specialized constraints.

CONTEMPORARY HISTORY

To illustrate some of the details involved in the atomistic computer-modelling techniques of plasmas, we consider the case of anomalous plasma diffusion studied by R. W. Hockney (5), an associate of O. Buneman. This problem is motivated by the difficulties encountered in containing plasma for thermonuclear fusion. Here, a special advance in tying together the individual particle trajectories is achieved by movie display.

A plasma consisting of electrons and positive ions is generated in an infinite cylinder with an isotropic Maxwellian velocity distribution. The problem is to investigate the diffusion of the particles to a surrounding concentric insulated wall under the guidance of a constant magnetic field parallel to the axis of the cylinder.

The trajectories of each of 1,000 charged particles is followed on the computer on the basis of a cyclic 5-step process: (1) The position and velocity of each particle is stored in the computer memory. (2) From the position of each charge, a charge distribution is inserted in Poisson's equation to obtain the electrostatic potential. (3) From the potential, the electric force on each charge is determined. (4) This force, plus the force on a charge due to the magnetic field, are inserted in Newton's equations. (5) These are solved for new positions and velocities after a short time step. The cycle is now back to (1) and ready to be repeated. Fig. 3 illustrates the individual paths of charges. Plasma contraints are chosen so that the paths are collisionless.

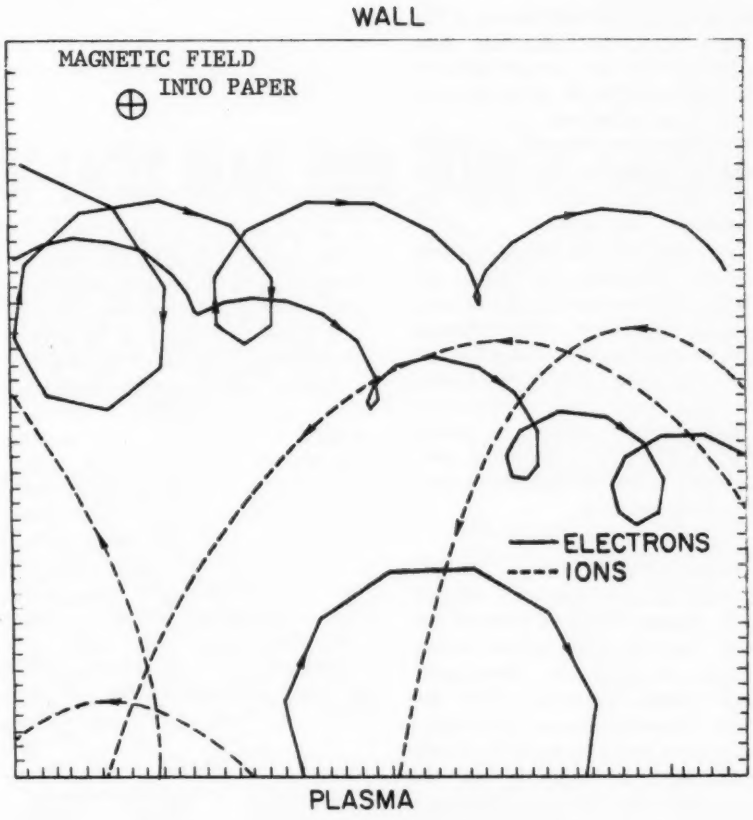

Figure 3.—Collisionless orbits in anomalous plasma diffusion (ref. 5).

A routine execution of this program within a reasonable time is beyond the capacity and speed of present-day computers. A trading between physically significant approximations and computer capacity becomes necessary. Thus, for example, the ratio of the mass of the proton to that of the electron is decreased by a factor of 30. In fact, the problem became practical only with the invention of a new direct technique for solving Poisson's equations using Fourier analysis. (5) It is more rapid by a factor of 10 than the previous iterative methods.

As noted, the results are displayed as a movie. Fig. 4 is a representative still frame. To obtain the illustrated rectangles, a cross section of the concentric cylinders is cut along a radius and stretched out into a rectangle. The side of the rectangle marked "plasma" represents the inner cylinder with the source of charged particles, and the side marked "wall" is the surrounding receiving cylinder. The upper left rectangle shows the distribution of charges, the upper right rectangle the flux of the charges, and the lower rectangle the potential distribution.

The main conclusion identified the existence of an anomalous diffusion of charges from the plasma to the wall. The succession of the movie frames shows a quasisteady state with no diffusion followed by the onset of a macroscopic plasma wave. This wave is the mechanism for the diffusion. The diffusion oscillates between a predominantly electron-transmitting state and a predominantly positive-ion-transmitting state. An electron-transmitting state and a quasisteady state are depicted in Figs. 4 and 5, respectively. The flux arrows identify Fig. 4 as an electron-transmitting state. The hump in the potential distribution of Fig. 4 identifies the plasma wave. This should be compared with the

quiescent potential distribution of Fig. 5 representing the quasisteady state. As pointed out, the particle paths are collisionless so that the diffusion is not of the usual collisional type. In fact, this collisionless diffusion is several orders of magnitude larger than collisional diffusion, which explains the designation, "anomalous."

In comparing the above atomistic computer modelling for plasma diffusion with previous more phenomenological approaches, two advantages might be mentioned: 1) Large Larmor radii*—i.e., comparable to the apparatus size—may be introduced. 2) Nonlinearities present no greater difficulty for the computer than linearities. In general, phenomenological analyses are linear.

FUTURE POSSIBILITIES

With the new generation of computers, bearing increased memory and speed, one can look forward to the solution of significant three-dimensional plasma problems. This will permit three-dimensional boundaries which are of special interest for plasma containment. In addition, one can envision more sophisticated displays to tackle the central hurdle of the many-body problem—the coherent grasp of the individual particle trajectories.

**A charged particle's motion is circular in a magnetic field. The radius of the circle is called the Larmor radius.*

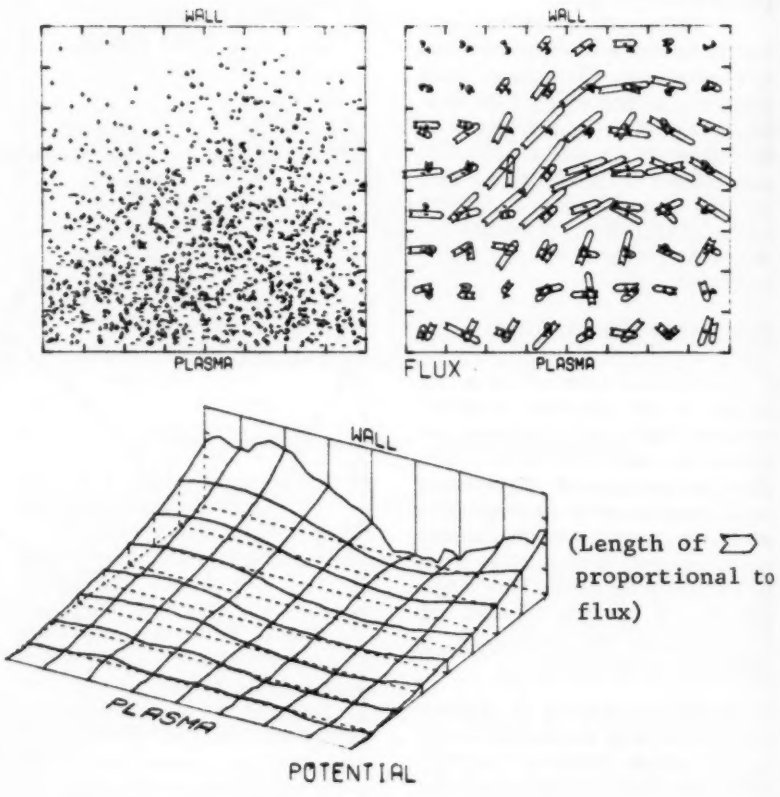

Figure 4.—An electron-transmitting state (ref. 5).

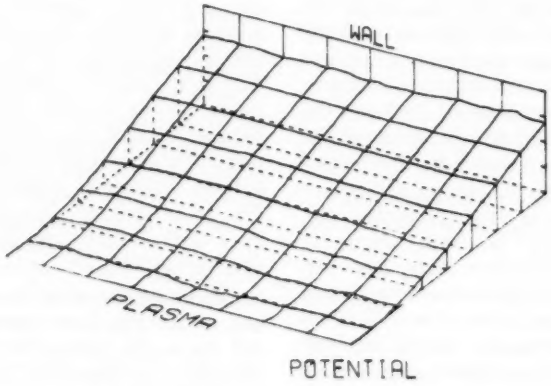

Figure 5.—Quasisteady state (ref. 5).

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DAYTIME REFLECTION OF LASER BEAM FROM GEODETIC SATELLITE

Although a laser beam has been reflected from a satellite many times at night, AFCRL geodesists, using the Explorer B (S-66) satellite as their target, have twice hit a satellite with a laser beam in daylight—the first known group in the world to succeed in doing so. The first success came on December 19, 1967, when they hit the target at a slant range of 1,109 km. They repeated the experiment on January 17, 1968. The Explorer B carries special reflectors for the laser equipment. The experiment itself is designed to improve geodetic measurements—that is, to obtain more accurate measurements of the distance between two widely separated points on the earth's surface, and improved knowledge of the size and shape of the earth.

The laser beam was fired by laser equipment located on the rooftop of AFCRL's main laboratory building. The reflected light was detected by a photomultiplier. Over the past several years, AFCRL has reflected a laser beam from a satellite at night many times. Success depends on precise calculations of orbital position and aiming point. Even with such calculations, atmospheric refraction is an unknown variable and can deflect the light beam.

The experimental multipulse ruby-crystal laser system used in the daytime experiments were designed by AFCRL and EG&G, Inc. The Q-switching of the laser is done by a Kerr cell and a polarizing prism. The laser, during a single pumping time of about 300 microseconds, transmits 5 pulses, each about 25 nanoseconds long, at approximately 1.5 joules per pulse output energy. AFCRL's earlier nighttime experiments were conducted with a normal pulsed mode laser. Satellites are the basis of several techniques being considered under the National Geodetic Satellite Program for use in the establishment of a worldwide network of ground stations in a common reference system relative to the center of the earth.

AFCRL's prototype geodetic laser equipment does not track satellites. It operates in a stationary mount with manually set elevation and azimuth angles. It is necessary, therefore, that the satellite elevation and azimuth and laser firing time be calculated with extreme accuracy. The necessary calculations were developed by George Hadgigeorge of AFCRL. The 9th Aerospace Defense Division, Ent AFB, Colorado, furnished satellite position and velocity on a predetermined epoch. The over-all experiment was under the direction of Robert L. Iliff.

TERRESTRIAL SCIENCES LABORATORY, AFCRL

Mr. George Hadgigeorge is a research geodesist with the Geodesy Branch, Terrestrial Sciences Laboratory, AFCRL. He was formerly employed by the Army Map Service, also as a geodesist. Presently, at AFCRL, he is responsible for planning and carrying out investigations in mathematical and astronomic geodesy to provide the mathematical research required in the Geodesy Branch's program of geodetic research, particularly in satellite areas.

Mr. Hadgigeorge received a B.A. in Mathematics from Norwich University, Northfield, Vermont, in 1960. He has several publications to his credit.

Fifth Coral Gables Conference on Symmetry Principles at High Energy

CAPT DONALD R. LEHMAN and DR. ERICH WEIGOLD
Directorate of Physical Sciences, AFOSR

The Fifth Coral Gables Conference on Symmetry Principles at High Energy was held recently at the Lowe Art Gallery on the University of Miami campus. This Conference, supported by the Nuclear Physics Division of AFOSR, was organized by Professor Behram Kursunoglu, Director of the Center for Theoretical Studies at the University of Miami.

In the opening talk of the Conference, Professor Melvin Schwartz of Stanford described a beautiful experiment his group had carried out at the Stanford Linear Accelerator on the charge asymmetric leptonic decay of the long-lived K° meson. Since this experiment was recently discussed at some length in this journal, we shall not elaborate on it here. (1) Besides discussing the significance of the experiment to charge conjugation–parity reversal (CP) violation in microscopic physics, Professor Schwartz also stressed the difficulty of accurately estimating the errors involved in such experiments. Although it is usually relatively easy to reduce the statistical errors, it is often much harder to allow for all the systematic errors that may be present. He warned the theoreticians not to take the experimental numbers with their quoted errors too seriously. Later in the program, William Willis of Yale University and W. Galbraith of the University of Sheffield also described experimental results in their talks. However, the main emphasis during the conference was on theory.

Abraham Pais of the Rockefeller University described how phase-shift information on pion-pion scattering and the pion-pion scattering lengths can be obtained without making any assumptions about strong interactions from the $K_{\ell 4}$ decays, such as $K^+ \to \pi^+ + \pi^- + \ell^+ + \nu$ where ℓ signifies a lepton (muon or electron). In addition to the lack of assumptions on the strong interaction dynamics, the weak interaction assumptions involved in the calculation are completely self-checking. Following Pais, Louis Michel of the Institut des Hautes Etudes Scientifiques, France, read a paper on the difficulties involved in using the electromagnetic or weak interactions to induce the observed semistrong breaking of SU_3 symmetry.

One talk of particular interest in regard to the theme of the conference was given by Lochlainn O'Raifeartaigh of the Institute for Advanced Study. The talk was entitled "Summary and Review of the History and Development of Combined Space-Time-Internal Symmetries." The major point of his presentation was that, no matter which approach one takes in the development of theories that include internal as well as space-time symmetries, there is a constant appearance of infinite component wave equations or, equivalently, of noncompact groups. Infinite component-wave equations have proved quite successful in the computation of mass spectra, electromagnetic form factors, and decay rates as well as for yielding a method for saturating current algebras at infinite momentum and providing the framework for making the quark model relativistic. Unfortunately, despite these successes, there are some problems with the theory. If one takes infinite component-wave equations very seriously and assumes they are good for all momenta and quantizes the fields, then difficulties arise at a fundamental level.

The papers of Bruno Zumino (New York University), Julian Schwinger (Harvard University), and Herman Munczek (Northwestern University) all dealt with the phenomenological Lagrangian approach to particle physics. This approach amounts to the construction of a Lagrangian with physical parameters to obtain dynamical results by means of perturbation theory. For instance, the technique has been used in an attempt to derive the mass difference between the charged and neutral pions. It reproduces most of the well-known results of current algebra as well as yielding a few new results.

Kazuhiko Nishijima of the University of Tokyo presented his model of CP violation. He introduced a neutral current, odd under the CP operator, into the weak interaction Hamiltonian. This current is postulated to be responsible for all nonleptonic decays of particles by second-order processes. The theory predicts certain values for the phenomenological parameters used to describe CP violation as well as the value of $\pm 2 \times 10^{-22}$ e-cm for the electric dipole moment of the nucleon. The next generation of experiments on CP violation should be able to test his predictions.

Altogether, 19 papers were read at the Conference, and there was a great deal of discussion. Professor Nicola Cabibbo of the Universita degli Studi, Roma, summarized the Conference in his paper entitled "New Ways in Symmetry and Dynamics." This was followed by a grand summary of the past 5 conferences on symmetries at high energies by Yuval Ne'eman of Tel Aviv University. Future conferences in this series will be of a somewhat wider scope and will be entitled "Fundamental Interactions at High Energy." The *Proceedings* of the Conference were to be published by W. A. Benjamin, Inc., and should be available this summer.

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TEMPERATURES AT SUPERSONIC AIRCRAFT ALTITUDES

AEROSPACE INSTRUMENTATION LABORATORY, AFCRL

At the cruise altitude of supersonic aircraft, between 60,000 and 80,000 feet, air temperature greatly affects the rate of fuel consumption. For example, the allowable payload of a supersonic transport on a 3,000-mile trip may be reduced by perhaps 9 passengers and their baggage when the average route temperature at cruising level is about 14 degrees C warmer than normal. ("Normal" is the standard temperature which, in the supersonic transport altitude region, is about -50 degrees C.)

For subsonic aircraft, many studies have been made of average preselected route temperatures by season and altitude. Few studies for supersonic aircraft altitudes have been made. From the standpoint of Air Force operations, such a study should provide a means for calculating the probability of upper-air temperature at relatively short notice for any route without recourse to current temperature data or lengthy calculations.

This need has led Irving I. Gringorten of AFCRL to develop a model whereby average temperatures for any randomly selected route over the North American continent can be calculated in a relatively simple manner. The model is purely statistical. The calculations do not require a knowledge of observed upper-air temperatures at any specified time. For the study, Gringorten used daily observations form 66 North American stations for a 5-year period.

No method for calculating route temperatures would be particularly noteworthy if it involved only the averaging of temperatures during a given season along a particular route. For greater precision, the calculations must depend on using a sufficient number of temperature checkpoints along the route and knowing not only the individual mean temperature and standard deviations of each checkpoint but also the correlation coefficients between pairs of checkpoints.

The correlation coefficients present the difficulty. To adequately cover the Northern Hemisphere, the tables that give such intercorrelations would have to be voluminous, to say nothing of the massive effort that would be required to produce them. The distinctive feature of the Gringorten model is that it yields useful and simple estimates of these correlation coefficients.

The key element of the model is a single parameter that can be assigned to each station individually so that it can yield a plot on a map in the same manner that temperature gradients are mapped. This parameter is a value that permits the calculations of correlation coefficients between one station and all other stations within a reasonable distance from it.

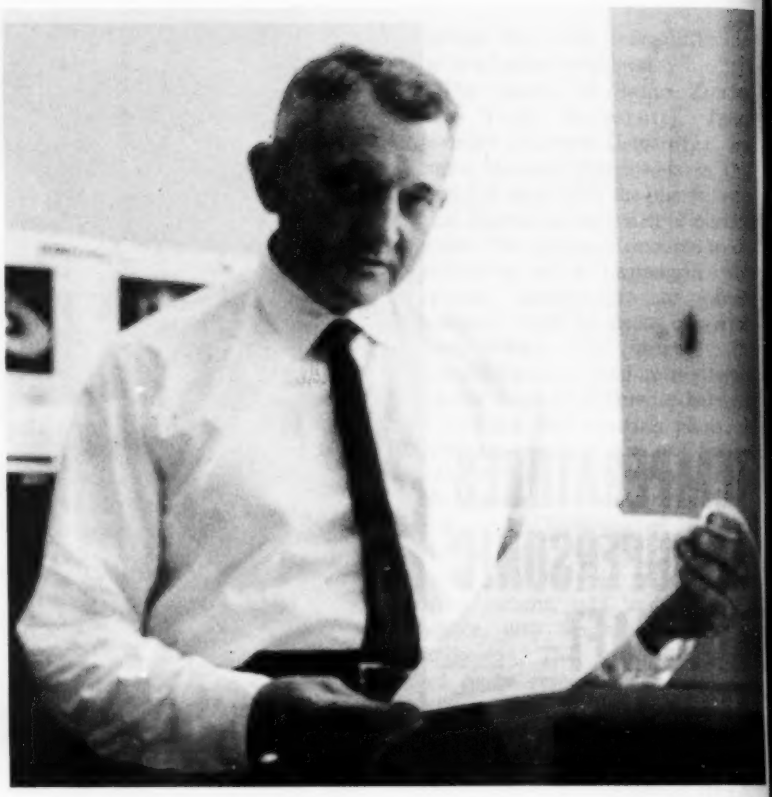
Just how this parameter is derived is an involved statistical process. The result, however, is a series of correlation coefficient isopleths (contour lines of equal value), by season and altitude, overlaying a map of the North American continent. These isopleths provide the user with one of the three essential parameters for calculating temperatures along a particular flight path. The other two parameters are mean temperature and

standard deviations, which are also plotted as isotherms and isopleths covering the North American continent. By applying the data given in an appropriate set of three of these maps to a relatively simple statistical formula, it is possible to estimate the relative frequencies of critical route temperatures.

The statistical model is presented in the AFCRL report, "A Statistical Model of the Temperature Field at Supersonic Aircraft Altitudes," (67-0274), by Irving I. Gringorten.

Mr. Irving I. Gringorten is a supervisory research meteorologist with the Design Climatology Branch, Aerospace Instrumentation Laboratory, AFCRL. He has been with AFCRL or its predecessor organizations since 1947, and is engaged in work on design climatology. Currently, he is devoting his time to the modelling of the aspects of duration and frequency of occurrence of weather events and their spatial distribution.

Mr. Gringorten has a B.A. in Physics and Geology (1935) and an M.A. in Meteorology (1936), both from the University of Toronto. He took advanced studies at the California Institute of Technology from 1937 to 1940. Mr. Gringorten is a member of the American Meteorological Society and the American Statistical Association.



RESEARCH IN THE ANDES

MAJ JOSEPH E. GORRELL
Directorate of Physical Sciences
AFOSR

Atop Mt. Chacaltaya in the thin, crisp atmosphere at 17,000 feet is situated the world's highest laboratory. This laboratory, a part of the Universidad Mayor de San Andrés, is only a few miles (about an hour's drive) outside the city of La Paz, Bolivia. Being near the equator, the laboratory has a relatively mild climate as compared to other mountaintop installations. The average wind velocity is approximately 15 mph, and the temperature is such that snow accumulations do not prevent access to the laboratory at any time of the year. This relatively mild climate, the high elevation, and the proximity to the geomagnetic equator make Mt. Chacaltaya a favorable location for conducting certain types of cosmic-ray experiments.

AFOSR is supporting several experiments at Mt. Chacaltaya. The major experiment is called the Bolivian Air Shower Joint Experiment (BASJE), which is a cooperative effort among universities in Bolivia, Japan, and the United States. Its original objective was to determine whether very-high-energy gamma rays are a constituent of the primary cosmic radiation that continually bombards the earth. The more recent objectives of this experiment include a study of the core structures of cosmic-ray showers and particle interactions at extremely high energies. Other experiments being conducted at Mt. Chacaltaya, under AFOSR sponsorship, include a study of the Cerenkov light emitted by cosmic-ray air showers as they traverse the atmosphere, an investigation of the radio pulses emitted by air showers, and a study of time variations of cosmic-ray intensity for both neutrons and charged particles.

Although conducting experiments at high elevations is not as easy as at sea level, the facilities at Mt. Chacaltaya are such as to make it more attractive than most mountaintop installations. The laboratory can accommodate about 20 people at one time, and has sufficient electrical power for experimental needs. In addition, much equipment from past experiments is available to scientists for new experiments. For these reasons, many investigators have found it worthwhile to conduct their research at Mt. Chacaltaya.

GPO 863-507